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LINEAR CONVERGENCE OF THE CONJUGATE GRADIENT METHOD*

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ABSTRACT: It is shown that the method of conjugate gradients for the minimization of a quadratic function converges no better than linearly if the standard starting and restarting procedures are not used.

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1. THE METHOD OF CONJUGATE GRADIENTS

The conjugate gradient method [1] is an efficient procedure for unconstrained optimization problems of the type

$$\text{minimize } f(x_1, x_2, \ldots, x_n)$$

where $f(x)$ is a suitable (differentiable, and preferably convex) function on E^n. In particular, if $f(x) = c + p^T x + \frac{1}{2} x^T Qx$ and Q is an n^{th} order symmetric and positive semidefinite matrix (thus $f(x)$ is convex), then the conjugate gradient method will terminate at the solution in at most n steps, provided the standard starting procedure is used. A statement of the conjugate gradient method for this function is:

Given x_0, let $d_0 = -\nabla f(x_0)$.

For $k > 0$, given x_k and d_k, let $x_{k+1} = x_k + t_k d_k$,

where t_k is the value of t minimizing $f(x_k + td_k)$.

If $\nabla f(x_{k+1}) = 0$, stop. Otherwise, let

$d_{k+1} = -\nabla f(x_{k+1}) + s_k d_k$,

where s_k is chosen so that $d_{k+1}^T Qd_k = 0$.

Let $g_k = \nabla f(x_k)$ for all k. Noting that

$$\begin{aligned} g_{k+1} &= \nabla f(x_{k+1}) \\ &= p^T + Q(x_k + t_k d_k) \\ &= p^T + Qx_k + t_k Qd_k \\ &= g_k + t_k Qd_k, \end{aligned}$$

we can write the recursion as:

$$d_0 = -g_0; \tag{1}$$

For $k > 0$,

$$\begin{aligned} g_{k+1} &= g_k + t_k Q d_k \\ d_{k+1} &= -g_{k+1} + s_k d_k \end{aligned} \tag{2}$$

$$\text{where } t_k = -g_{k+1}^T d_k / d_k^T Q d_k \tag{3}$$

$$\text{and} \quad s_k = g_{k+1}^T Q d_k / d_k^T Q d_k \tag{4}$$

$$\text{or} \quad s_k = g_{k+1}^T (g_{k+1} - g_k) / d_k^T (g_{k+1} - g_k). \tag{5}$$

The formula (5) for s_k is essentially formula (3:2b) of Hestenes and Stiefel, rather than the more commonly used formula (3:1e), which in our notation is $s_k = g_{k+1}^2 / g_k^2$. As they subsequently show, the former gives better protection against the accumulation of roundoff error. More importantly, it ensures that $d_{k+1}^T Q d_k = 0$ for each k, independently of whether the other steps have been carried out accurately, which the latter formula does not. If all the needed relations do hold accurately, it can be shown that the successive directions $d_0, d_1, \ldots$ are all linearly independent and conjugate (that is, $d_j^T Q d_k = 0$ for $j \neq k$), and that x_k minimizes the function f on the affine set passing through x_0 and spanned by $d_0\ d_1, \ldots, d_{k-1}$. Consequently the procedure must terminate with $g_k = 0$ for some $k \leq n$.

2. THE PROBLEM

It is important to note that both the starting condition (1) and the determinations (3, 4) of the coefficients t_k and s_k must be observed precisely in order that

the above termination ensues; it cannot be shown otherwise. Indeed, failure to choose a "standard start"--one in which d_0 is parallel to g_0--makes it impossible to retain the conjugancy relation $d_j^T Q d_k = 0$ for $|j-k| \neq 1$ using formulas of the type of (2). (We have seen this fact overlooked in some reports in the literature, leading to an overestimate of the convergence rate of the method.) Since, however, the procedure is almost invariably used under circumstances in which the condition $g_k = 0$ cannot be precisely met-- with the quadratic problem in an environment of roundoff error, and, more significantly, in extensions of the method to nonquadratic problems, such as that due to Fletcher and Reeves [2] -- provision for continuing after the n^{th} step must be made. It has generally been recognized as good practice to restart the procedure after n (or possibly $n+1$ or $n+2$) iterations; that is, to begin all over again, using the latest point x_k found as the new x_0, and thus rebuild a new set of conjugate directions.

The purpose of the study described here was to determine whether restarting was, in fact, necessary, or whether the procedure could be continued indefinitel without restarting and not suffer. We have concluded that restarting is necessary for quick convergence. Indeed, we have an example (for n=3) of a quadratic problem which shows that convergence can be no better than linear when a nonstandard start is used (while, of course, a standard start or restart would cause termination in at most three iterations).

3. THE EXAMPLE: CONVERGENCE IS AT BEST LINEAR

We have run about fifty steps of the continued conjugate gradient method as defined by equations (2-4) above on each of some one hundred quadratic, three-variable problems, examining graphically the ratios $f(x_{k+1})/f(x_k)$ of successive values of the function $f(x) = \frac{1}{2}x^TQx$. In about half of the trials, Q was the diagonal matrix whose eigenvalues are $(0.1, 1, 1)$; the starting vectors g_0 and d_0 were chosen randomly. In every case the ratios, while first seemingly randomly scattered between 0 and 1, were found to lie in a rather definitely marked interval $[a, b]$ with $0 < a < b < 1$. In many cases it appeared that something very much like a sine curve having a period between three and five steps could be fitted to the set of successive ratios. After considerable experimentation with the starting data, we found an example in which the ratios were constant. The other data of the procedure then exhibited a remarkable periodicity, and the discovery of simple relationships among these led to the following example:

$$\text{let } Q = \begin{bmatrix} 0.1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$g_0 = (1, \; -\sqrt{5}, \; 0)^T / \sqrt{6}$$

$$d_0 = (-10\sqrt{5}, \; 14, \; -3\sqrt{6})^T / 4\sqrt{30}$$

One step of the method given by equations (2-4) is

$$g_{k+1} = g_k + t_k Q d_k$$

$$d_{k+1} = -g_{k+1} + s_k d_k .$$

In our case $t_k = -8/5$, and $s_k = 9/25$ for all k.

Furthermore, the relations

$$g_{k+1} = rRg_k \text{ and}$$

$$d_{k+1} = rRd_k$$

hold for all k where $r = 3/5$ and R is the orthogonal matrix

$$R = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1/5 & -(2\sqrt{6})/5 \\ 0 & (2\sqrt{6})/5 & -1/5 \end{bmatrix} .$$

Thus $g_k = (rR)^k g_0$ and $d_k = (rR)^k d_0$ for all k. Each successive application of the matrix rR rotates the gradient and the direction through an angle arccos $(-1/5)$ around the long axis of the three-dimensional ellipsoid $x^T Qx = 1$, and diminishes both of these vectors in magnitude by the factor $r = 3/5$. Thus the ratio $f(x_{k+1})/f(x_k)$ is $9/25$ for all k.

4. THEOREM: CONVERGENCE IS AT WORST LINEAR

To bound the rate of convergence of the nonrestarted conjugate gradient method from both sides, we will show that its convergence is at worst linear.

Let $f(x) = \frac{1}{2}x^T Qx$ (we can always transform the original problem so that it has this form). Since $g = \nabla f(x) = Qx$, $f(x) = \frac{1}{2}g^T Q^{-1} g$. The minimum of f along any line $x + td$ is given by $t = \hat{t} = -g^T d/d^T Qd$ (compare with formula (3), suppressing "k"). Setting $x_+ = x + \hat{t}d$ and $g_+ = \nabla f(x_+)$, we have

$$2f(x_+) = g_+^T Qg_+ = (g + \hat{t}Qd)^T Q^{-1}(g + \hat{t}Qd) = gQ^{-1}g - (g^T d)^2/d^T Qd.$$

We consider two cases:

(i) $d = -g$; that is, the step is an ordinary steepest descent step.

Then

$$2f(x_+) = g^T Q^{-1} g - (g^T g)^2 / g^T Q g.$$

(ii) The point x was obtained by minimizing f along some line having the direction c, whence $g^T c = 0$, and then the direction d was obtained as in formulas (2,4), so that

$$d = -g + sc \text{ and } d^T Q c = 0.$$

Then $g^T d = 0 - g^T g$ and

$$d^T Q d = -g^T Q d = -g^T(-Qg + sQc) = g^T Q g - s g^T Q c$$
$$= g^T Q g - (g^T Q c)^2 / c^T Q c.$$

We see that $d^T Q d \leq g^T Q g$.

Since in case (ii) $2f(x_+) = g^T Q^{-1} g - (g^T g)^2 / d^T Q d$, the resulting value of f is no higher in case (ii) than in case (i); the fact that the direction d was obtained by conjugating $-g$ with respect to the previous direction, rather than taking it to be $-g$ itself, has not hurt. Thus each step of the continued conjugate gradient method decreases the function at least as much as would one step of steepest descent taken at the same point. The inequality

$$f(x_{k+1}) / f(x_k) \leq (A-1/A+1)^2$$

is known to hold for steepest descent, where A is the condition number of the matrix Q (namely, the ratio of the largest to smallest eigenvalue).

It follows that the inequality also holds for the conjugate gradient method, so that its convergence is at worst linear.

REFERENCES

[1] M. R. Hestenes and E. Stiefel, 1952, "Methods of Conjugate Gradients for Solving Linear Systems", J. Res. NBS 49, 409-436.

[2] R. Fletcher and C. M. Reeves, 1964, "Function Minimization by Conjugate Gradients", Computer J. 7, 149-154.